=>
Uploading C:\Program Files\Stnexp\Queries\10578800\reaction VI to I.str

chain nodes :
6   7   8   9   10   11   12   13   14   20   21   22   23   24   25   26   27   28   29   30   31   32   33   34   35
ring nodes :
1   2   3   4   5   15   16   17   18   19
chain bonds :
1-7   3-31   5-6   6-10   7-8   7-9   7-12   9-11   10-14   10-35   11-13   11-34   15-23   17-20   19-22   20-21
22-26   23-24   23-25   23-28   25-27   26-30   26-33   27-29   27-32
ring bonds :
1-2   1-5   2-3   3-4   4-5   15-16   15-19   16-17   17-18   18-19
exact/norm bonds :
1-2   1-5   2-3   3-4   4-5   5-6   6-10   7-9   9-11   10-14   11-13   15-16   15-19   16-17   17-18   17-20   18-19
19-22   22-26   23-25   25-27   26-30   27-29
exact bonds :
1-7   3-31   7-8   7-12   10-35   11-34   15-23   20-21   23-24   23-28   26-33   27-32

Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:CLASS   7:CLASS   8:CLASS   9:CLASS   10:CLASS   11:CLASS   12:CLASS
 13:CLASS   14:CLASS   15:Atom   16:Atom   17:Atom   18:Atom   19:Atom   20:CLASS   21:CLASS   22:CLASS   23:CLASS
 24:CLASS   25:CLASS   26:CLASS   27:CLASS   28:CLASS   29:CLASS   30:CLASS   31:CLASS   32:CLASS   33:CLASS
34:CLASS   35:CLASS
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:
containing 15

L1   STRUCTURE UPLOADED

=> s l1
SAMPLE SEARCH INITIATED 17:52:40 FILE 'CASREACT'
SCREENING COMPLETE -   1 REACTIONS TO VERIFY FROM   1 DOCUMENTS

100.0% DONE   1 VERIFIED   0 HIT RXNS   0 DOCS
SEARCH TIME: 00.00.01

```
FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED VERIFICATIONS:        1 TO        79
PROJECTED ANSWERS:              0 TO         0


L2              0 SEA SSS SAM L1 (      0 REACTIONS)

=> s l1 full
FULL SEARCH INITIATED 17:52:43 FILE 'CASREACT'
SCREENING COMPLETE -     144 REACTIONS TO VERIFY FROM        86 DOCUMENTS

100.0% DONE    144 VERIFIED       0 HIT RXNS                    0 DOCS
SEARCH TIME: 00.00.01

L3              0 SEA SSS FUL L1 (      0 REACTIONS)

=> file stng
COST IN U.S. DOLLARS                             SINCE FILE      TOTAL
                                                   ENTRY        SESSION
FULL ESTIMATED COST                               113.55        113.76


FILE 'STNGUIDE' ENTERED AT 17:52:52 ON 12 JUN 2007
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FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Jun  8, 2007 (20070608/UP).

=> file casreact
COST IN U.S. DOLLARS                             SINCE FILE      TOTAL
                                                   ENTRY        SESSION
FULL ESTIMATED COST                                0.12         113.88

FILE 'CASREACT' ENTERED AT 17:53:48 ON 12 JUN 2007
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
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held by the publishers listed in the PUBLISHER (PB) field (available
for records published or updated in Chemical Abstracts after December
26, 1996), unless otherwise indicated in the original publications.

FILE CONTENT:1840 - 9 Jun 2007 VOL 146 ISS 25

New CAS Information Use Policies, enter HELP USAGETERMS for details.

************************************************************
*                                                          *
*      CASREACT now has more than 12 million reactions     *
*                                                          *
************************************************************

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999)
provided by InfoChem, INPI data prior to 1986, and Biotransformations
database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance
identification.

=>
Uploading C:\Program Files\Stnexp\Queries\10578800\reaction VI to I acyl.str
```
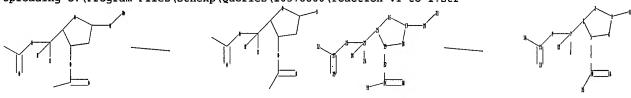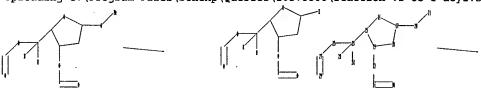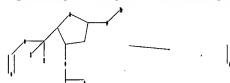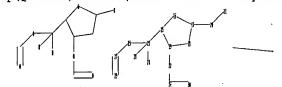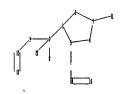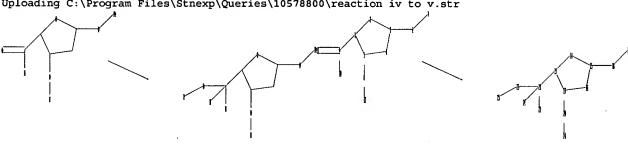
```
chain nodes :
6  7  8  9  10  11  12  13  14  20  21  22  23  24  25  26  27  28  29  30  31
ring nodes :
1  2  3  4  5  15  16  17  18  19
chain bonds :
1-7  3-31  5-6  6-10  7-8  7-9  7-12  9-11  10-14  11-13  15-23  17-20  19-22  20-21  22-26  23-24
23-25  23-28  25-27  26-30  27-29
```

ring bonds :
1-2 1-5 2-3 3-4 4-5 15-16 15-19 16-17 17-18 18-19
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5 5-6 6-10 7-9 9-11 10-14 11-13 15-16 15-19 16-17 17-18 17-20 18-19
19-22 22-26 23-25 25-27 26-30 27-29
exact bonds :
1-7 3-31 7-8 7-12 15-23 20-21 23-24 23-28

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS
13:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:CLASS 21:CLASS 22:CLASS 23:CLASS
24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS

L4   STRUCTURE UPLOADED

=> d
L4 HAS NO ANSWERS
L4   STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s l4
SAMPLE SEARCH INITIATED 17:54:10 FILE 'CASREACT'
SCREENING COMPLETE -   70 REACTIONS TO VERIFY FROM   18 DOCUMENTS

100.0% DONE   70 VERIFIED   0 HIT RXNS   0 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED VERIFICATIONS: 899 TO   1901
PROJECTED ANSWERS: 0 TO   0

L5   0 SEA SSS SAM L4 (0 REACTIONS)

=> s l4 full
FULL SEARCH INITIATED 17:54:13 FILE 'CASREACT'
SCREENING COMPLETE -   4637 REACTIONS TO VERIFY FROM   461 DOCUMENTS

100.0% DONE   4637 VERIFIED   64 HIT RXNS   28 DOCS
SEARCH TIME: 00.00.01

L6   28 SEA SSS FUL L4 (64 REACTIONS)

=> d l6 1-28

L6   ANSWER 1 OF 28   CASREACT   COPYRIGHT 2007 ACS on STN

RX(86) OF 183 - 5 STEPS

1. Ac2O, H2SO4, Water,
   AcOH
2. HBr, Water, CH2Cl2
3.1. SO2Cl2, CH2Cl2,
     DMF
3.2. 1H-Imidazole
4. KHF2, HF,
   S:123513-85-9,
   Water
5. HBr, AcOH, CH2Cl2

REF: Faming Zhuanli Shenqing Gongkai Shuomingshu, 1891710, 10 Jan
      2007

NOTE: 2) regioselective, 4) stereoselective, 5) regioselective, in the
      dark
CON: STEP(1.1) 0 deg C; 0 deg C -> room temperature; overnight,
           cooled
      STEP(2.1) 3.5 hours, 0 deg C; 2 hours, room temperature
      STEP(3.1) -15 deg C; 0.5 hours, -15 deg C;
           -15 deg C -> room temperature; 4 hours, room temperature
      STEP(3.2) 0 deg C; 17 hours, room temperature
      STEP(4.1) room temperature -> 150 deg C; 150 deg C -> 160 deg C;
           1 hour, 160 deg C
      STEP(5) 24 hours, room temperature

RX(35) OF 806

1. MeOCHCl2, SnCl4,
   CH2Cl2
   ————————————————→
2. Water

     REF: Journal of Organic Chemistry, 71(21), 8071-8088; 2006
·NOTE: regioselective
CON: STAGE(1) 13 hours, room temperature
       STAGE(2) 45 minutes, room temperature

RX(1) OF 17

PBr3, ZnBr2, CHCl3
————————————————→

RX(1) OF 17

                    48%
REF: Eur. Pat. Appl., 1705181, 27 Sep 2006
CON: 19 hours, 45 deg C

RX(2) OF 21

1. HCl, Water,
   Dioxane
2. DAST [(Et2N).SF3],
   THF
3. MeOH

(step 1)

53%

REF: Journal of the American Chemical Society, 127(44), 15612-15617;
       2005

CON: STAGE(1) 1 hour, reflux
       STAGE(2) -78 deg C; 20 minutes, room temperature
       STAGE(3) room temperature

RX(2) OF 33

HCl, Et2O

72%

REF: Organic Letters, 7(14), 2853-2856; 2005

NOTE: stereoselective
CON: 10 minutes, 0 deg C

REF: Faming Zhuanli Shenqing Gongkai Shuomingshu, 1539845, 27 Oct
      2004
CON: 2 - 4 hours, 30 deg C

L6   ANSWER 7 OF 28   CASREACT   COPYRIGHT 2007 ACS on STN

90%

REF: PCT Int. Appl., 2005044832, 19 May 2005

CON: STAGE(1) room temperature; room temperature -> 5 deg C;
         <15 deg C; 1 hour, 5 deg C

L6   ANSWER 8 OF 28   CASREACT   COPYRIGHT 2007 ACS on STN

AcCl, MeOH

REF: U.S. Pat. Appl. Publ., 2004266996, 30 Dec 2004
NOTE: workup
CON: STAGE(1) room temperature; room temperature -> 10 deg C;
      3.5 - 4 hours, 8 - 10 deg C; 4 hours, 8 - 10 deg C

L6   ANSWER 9 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

AcOH, AcCl

79%

REF: Organic & Biomolecular Chemistry, 1(13), 2267-2275; 2003

NOTE: stereoselective
CON: room temperature

L6   ANSWER 10 OF 28 CASREACT COPYRIGHT 2007 ACS on STN

MeO ... Me

HCl, AcOH→

Cl ... Me

72%

REF: Organic Letters, 4(26), 4571-4574; 2002
CON: STAGE(1) 5 minutes, room temperature; 1 hour, 10 deg C

L6   ANSWER 11 OF 28   CASREACT   COPYRIGHT 2007 ACS on STN

MeO AcO OAc Me

HBr, AcOH→

Br AcO OAc Me

REF: Tetrahedron Letters, 43(37), 6553-6555; 2002
CON: 1 - 3 hour, 20 deg C

L6   ANSWER 12 OF 28   CASREACT   COPYRIGHT 2007 ACS on STN

RX(57) OF 206 - 3 STEPS

1. F3CCO2H, Water
2. Ac2O, Pyridine
3. HBr, AcOH

REF: Nucleosides, Nucleotides & Nucleic Acids, 20(4-7), 747-750;
2001
NOTE: 1) stereoselective, 2:1 alpha:beta, 2) stereoselective, 3:1
alpha:beta, 3) stereoselective, 6:1 alpha:beta

L6   ANSWER 13 OF 28   CASREACT   COPYRIGHT 2007 ACS on STN

RX(62) OF 180 - 3 STEPS

1.1. F3CCO2H, Water
1.2. NaHCO3, Water
2. Ac2O, Pyridine
3. HBr, CH2Cl2, AcOH

stereoisomers

REF: Nucleosides, Nucleotides & Nucleic Acids, 20(8), 1583-1598;
2001
NOTE: 1) 67:33 alpha:beta, stereoselective, 2) stereoselective, 3)
86:14 alpha:beta, stereoselective

L6   ANSWER 14 OF 28   CASREACT   COPYRIGHT 2007 ACS on STN

1. HCl,
   Isopropyl ether
2. AcCl

(step 1)

85%

REF: Jpn. Kokai Tokkyo Koho, 2000290289, 17 Oct 2000

L6   ANSWER 15 OF 28   CASREACT   COPYRIGHT 2007 ACS on STN

HCl, AcOH

39%

REF: European Journal of Organic Chemistry, (5), 861-866; 2000

NOTE: gaseous HCl used
CON: STAGE(1) 0 deg C; 10 minutes

L6   ANSWER 16 OF 28   CASREACT   COPYRIGHT 2007 ACS on STN

AcCl, MeOH,
Cyclohexane

stereoisomers

REF: Jpn. Kokai Tokkyo Koho, 07224081, 22 Aug 1995, Heisei
NOTE: 25.degree. for 4 h; 84.8% yield

L6   ANSWER 17 OF 28   CASREACT   COPYRIGHT 2007 ACS on STN

HCl, Isopropyl ether

REF: Eur. Pat. Appl., 635517, 25 Jan 1995

L6   ANSWER 18 OF 28   CASREACT   COPYRIGHT 2007 ACS on STN

stereoisomers   stereoisomers

REF: PCT Int. Appl., 9310137, 27 May 1993
NOTE: 2 STEPS

L6   ANSWER 19 OF 28   CASREACT   COPYRIGHT 2007 ACS on STN

HCl, AcOH

stereoisomers

60%

REF: Tetrahedron, 43(18), 4227-34; 1987

L6   ANSWER 20 OF 28   CASREACT   COPYRIGHT 2007 ACS on STN

HCl, AcOH

stereoisomers

83%

REF: Tetrahedron, 43(10), 2355-68; 1987

L6   ANSWER 21 OF 28   CASREACT   COPYRIGHT 2007 ACS on STN

HCl, Isopropyl ether

REF: Nippon Kagaku Kaishi, (12), 1765-70; 1986

L6   ANSWER 22 OF 28   CASREACT   COPYRIGHT 2007 ACS on STN

RX(6) OF 177

77%

REF: Tetrahedron, 42(19), 5427-41; 1986

L6   ANSWER 23 OF 28   CASREACT   COPYRIGHT 2007 ACS on STN

RX(3) OF 5

REF: Eur. Pat. Appl., 145978, 26 Jun 1985

RX(2) OF 3

MeO

AcBr→

RX(2) OF 3

Br

REF: U.S., 4282349, 04 Aug 1981

RX(1) OF 51

MeO

Me

HCl→

Me

Cl

Me

Me

66%

REF: U.S., 4239753, 16 Dec 1980

HBr, CH2Cl2 →

68%

REF: Carbohydrate Research, 47(2), 233-40; 1976
NOTE: Classification: Substitution; Bromination; # Conditions: HBr
      CH2Cl2; 24h 0-3 deg

L6   ANSWER 27 OF 28   CASREACT   COPYRIGHT 2007 ACS on STN

HCl, AcOH, Et2O →

65%

REF: Journal of the American Chemical Society, 83,, 4066-50; 1961

NOTE: Classification: Substitution; Chlorination; # Conditions: HCl
      Et2O AcOH

L6   ANSWER 28 OF 28   CASREACT   COPYRIGHT 2007 ACS on STN

HCl, AcOH

70%

REF: Journal of the American Chemical Society, 81,, 4112-13; 1959

NOTE: Classification: Substitution; Chlorination; # Conditions: HCl
AcOH

```
=> d his

     (FILE 'HOME' ENTERED AT 17:52:00 ON 12 JUN 2007)

     FILE 'CASREACT' ENTERED AT 17:52:11 ON 12 JUN 2007
L1              STRUCTURE UPLOADED
L2          0 S L1
L3          0 S L1 FULL

     FILE 'STNGUIDE' ENTERED AT 17:52:52 ON 12 JUN 2007

     FILE 'CASREACT' ENTERED AT 17:53:48 ON 12 JUN 2007
L4              STRUCTURE UPLOADED
L5          0 S L4
L6         28 S L4 FULL

=>

---Logging off of STN---


=>
Executing the logoff script...

=> LOG Y
```

COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                ENTRY   SESSION
FULL ESTIMATED COST   194.08   307.96

STN INTERNATIONAL LOGOFF AT 17:54:44 ON 12 JUN 2007

=>
Uploading C:\Program Files\Stnexp\Queries\10578800\reaction VI to I acyl.str

chain nodes :
6   7   8   9   10 11 12 13 14 20 21 22 23 24 25 26 27 28 29 30 31
ring nodes :
1   2   3   4   5   15 16 17 18 19
chain bonds :
1-7   3-31   5-6   6-10   7-8   7-9   7-12   9-11   10-14   11-13   15-23   17-20   19-22   20-21   22-26   23-24
23-25   23-28   25-27   26-30   27-29
ring bonds :
1-2   1-5   2-3   3-4   4-5   15-16   15-19   16-17   17-18   18-19
exact/norm bonds :
1-2   1-5   2-3   3-4   4-5   5-6   6-10   7-9   9-11   10-14   11-13   15-16   15-19   16-17   17-18   17-20   18-19
19-22   22-26   23-25   25-27   26-30   27-29
exact bonds :
1-7   3-31   7-8   7-12   15-23   20-21   23-24   23-28

Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:CLASS   7:CLASS   8:CLASS   9:CLASS   10:CLASS   11:CLASS   12:CLASS
13:CLASS   14:CLASS   15:Atom   16:Atom   17:Atom   18:Atom   19:Atom   20:CLASS   21:CLASS   22:CLASS   23:CLASS
24:CLASS   25:CLASS   26:CLASS   27:CLASS   28:CLASS   29:CLASS   30:CLASS   31:CLASS

L1   STRUCTURE UPLOADED

=> s l1 full
FULL SEARCH INITIATED 17:59:29 FILE 'CASREACT'
SCREENING COMPLETE -   4637 REACTIONS TO VERIFY FROM   461 DOCUMENTS

100.0% DONE   4637 VERIFIED   64 HIT RXNS   28 DOCS
SEARCH TIME: 00.00.01

L2   28 SEA SSS FUL L1 (64 REACTIONS)

=>
Uploading C:\Program Files\Stnexp\Queries\10578800\reaction V to VI.str

```
chain nodes :
6  7  8  9  10  11  12  13  14  15  16  22  23  24  25  26  27  28  29  30
ring nodes :
1  2  3  4  5  17  18  19  20  21
chain bonds :
1-9  3-6  5-8  6-7  8-12  9-10  9-11  9-14  11-13  12-16  13-15  17-25  19-22  21-24  22-23  24-28
25-26  25-27  25-30  27-29
ring bonds :
1-2  1-5  2-3  3-4  4-5  17-18  17-21  18-19  19-20  20-21
exact/norm bonds :
1-2  1-5  2-3  3-4  3-6  4-5  5-8  8-12  9-11  11-13  12-16  13-15  17-18  17-21  18-19  19-20  19-22
20-21  21-24  25-27
exact bonds :
1-9  6-7  9-10  9-14  17-25  22-23  24-28  25-26  25-30  27-29


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:CLASS  7:CLASS  8:CLASS  9:CLASS  10:CLASS  11:CLASS  12:CLASS
 13:CLASS  14:CLASS  15:CLASS  16:CLASS  17:Atom  18:Atom  19:Atom  20:Atom  21:Atom  22:CLASS  23:CLASS
 24:CLASS  25:CLASS  26:CLASS  27:CLASS  28:CLASS  29:CLASS  30:CLASS
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:
containing 17




L3      STRUCTURE UPLOADED

=> s l3
SAMPLE SEARCH INITIATED 17:59:52 FILE 'CASREACT'
SCREENING COMPLETE -      581 REACTIONS TO VERIFY FROM       45 DOCUMENTS

100.0% DONE     581 VERIFIED       2 HIT RXNS                    2 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED VERIFICATIONS:     10175 TO     13065
PROJECTED ANSWERS:              2 TO       124

L4            2 SEA SSS SAM L3 (     2 REACTIONS)

=> s l3 full
FULL SEARCH INITIATED 17:59:55 FILE 'CASREACT'
SCREENING COMPLETE -    11450 REACTIONS TO VERIFY FROM      894 DOCUMENTS

100.0% DONE   11450 VERIFIED      66 HIT RXNS                   43 DOCS
SEARCH TIME: 00.00.01

L5           43 SEA SSS FUL L3 (    66 REACTIONS)

=> d his

     (FILE 'HOME' ENTERED AT 17:59:06 ON 12 JUN 2007)

     FILE 'CASREACT' ENTERED AT 17:59:12 ON 12 JUN 2007
L1              STRUCTURE UPLOADED
L2          28 S L1 FULL
L3              STRUCTURE UPLOADED
L4           2 S L3
L5          43 S L3 FULL

=> s l2 and l5
L6          13 L2 AND L5
```

L6   ANSWER 1 OF 13   CASREACT   COPYRIGHT 2007 ACS on STN

RX(2) OF 183

PhCOCl, Pyridine

REF: Faming Zhuanli Shenqing Gongkai Shuomingshu, 1891710, 10 Jan
       2007
CON: STAGE(1) 0 deg C; 17 hours, room temperature

L6   ANSWER 2 OF 13   CASREACT   COPYRIGHT 2007 ACS on STN

RX(3) OF 21

1. 4-ClC6H4COCl
2. Water, CH2Cl2

(step 1)

REF: Faming Zhuanli Shenqing Gongkai Shuomingshu, 1539845, 27 Oct
       2004
CON: STAGE(1) 4 - 5 hours, 40 deg C
       STAGE(2) 0.5 hours, 5 - 10 deg C

L6   ANSWER 3 OF 13   CASREACT   COPYRIGHT 2007 ACS on STN

RX(4) OF 24

4-MeC6H4COCl, Et3N,
PhMe

89%

REF: PCT Int. Appl., 2005044832, 19 May 2005
CON: STAGE(1) room temperature -> 40 deg C; 40 deg C -> 60 deg C;
       5 hours, 60 deg C

RX(2) OF 34

85%

REF: Organic Letters, 4(26), 4571-4574; 2002
CON: STAGE(1) 0 deg C; overnight, room temperature

RX(8) OF 206

REF: Nucleosides, Nucleotides & Nucleic Acids, 20(4-7), 747-750;
       2001
NOTE: stereoselective

RX(8) OF 180

(step 1)

95%

REF: Nucleosides, Nucleotides & Nucleic Acids, 20(8), 1583-1598;
       2001

MeO—[ring: O, ^{13}C, H, ^{13}C, H, HO]—OH → 4-MeC6H4COCl, Pyridine

[structure: MeO—ring with ^{13}C—H, ^{13}C—H, two 4-methylbenzoate ester groups, Me, Me]

100%

REF: European Journal of Organic Chemistry, (5), 861-866; 2000
CON: 2 hours, 40 deg C

L6   ANSWER 8 OF 13   CASREACT   COPYRIGHT 2007 ACS on STN

MeO—[ring: O]—OH, OH → 1. 4-ClC6H4COCl, Pyridine 2. MeOH

(step 1)

[structure: MeO—ring with OH, O-benzoate groups bearing Cl]

REF: Eur. Pat. Appl., 635517, 25 Jan 1995

L6   ANSWER 9 OF 13   CASREACT   COPYRIGHT 2007 ACS on STN

MeO—[ring: O]—O—Ph, F, O—Ph → Br—[ring: O]—O—Ph, F, O—Ph

stereoisomers   stereoisomers

REF: PCT Int. Appl., 9310137, 27 May 1993
NOTE: 2 STEPS

L6   ANSWER 10 OF 13   CASREACT   COPYRIGHT 2007 ACS on STN

stereoisomers

$$\xrightarrow[\text{Pyridine}]{\text{4-MeC6H4COCl,}}$$

stereoisomers

REF: Tetrahedron, 43(18), 4227-34; 1987
NOTE: 87% overall

L6   ANSWER 11 OF 13   CASREACT   COPYRIGHT 2007 ACS on STN

$$\xrightarrow{\text{HCl, Isopropyl ether}}$$

REF: Nippon Kagaku Kaishi, (12), 1765-70; 1986

L6   ANSWER 12 OF 13   CASREACT   COPYRIGHT 2007 ACS on STN

MeO.⟨furanose ring⟩OH

HO   OH

4-O2NC6H4COCl →

MeO.⟨furanose ring structure with ester groups⟩

REF: U.S., 4282349, 04 Aug 1981

L6   ANSWER 13 OF 13 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 13

MeO⟨furanose ring structure with two 4-chlorobenzoate ester groups⟩Cl

HCl, AcOH, Et2O →

Cl⟨furanose ring structure with two 4-chlorobenzoate ester groups⟩Cl

65%

REF: Journal of the American Chemical Society, 83,, 4066-50; 1961

NOTE: Classification: Substitution; Chlorination; # Conditions: HCl
      Et2O AcOH

=>

---Logging off of STN---

=>
Executing the logoff script...

=> LOG Y

=>
Uploading C:\Program Files\Stnexp\Queries\10578800\reaction II to III.str

chain nodes :
7 8 9 10 11 12 13 14 15 21 22 23 24 25 26 27 28 29 30
ring nodes :
1 2 3 4 5 6 16 17 18 19 20
chain bonds :
2-8 3-9 4-10 6-7 7-12 8-13 9-14 10-11 11-15 16-24 18-21 20-23 21-22 23-30 24-25 24-27
25-26 26-29 27-28
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-20 17-18 18-19 19-20
exact/norm bonds :
1-2 1-6 2-3 2-8 3-4 3-9 4-5 5-6 6-7 10-11 16-17 16-20 17-18 18-19 18-21 19-20 20-23
24-27 25-26
exact bonds :
4-10 7-12 8-13 9-14 11-15 16-24 21-22 23-30 24-25 26-29 27-28

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS
13:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:CLASS 22:CLASS 23:CLASS
24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
fragments assigned product role:
containing 16
fragments assigned reactant/reagent role:
containing 1

L1   STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS
L1   STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 15:45:15 FILE 'CASREACT'
SCREENING COMPLETE -   522 REACTIONS TO VERIFY FROM   17 DOCUMENTS

100.0% DONE   522 VERIFIED   0 HIT RXNS   0 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED VERIFICATIONS: 9070 TO   11810
PROJECTED ANSWERS: 0 TO   0

L2   0 SEA SSS SAM L1 (0 REACTIONS)

=> s l1 full
FULL SEARCH INITIATED 15:45:23 FILE 'CASREACT'
SCREENING COMPLETE -   7531 REACTIONS TO VERIFY FROM   254 DOCUMENTS

100.0% DONE   7531 VERIFIED   6 HIT RXNS   3 DOCS
SEARCH TIME: 00.00.02

L3   3 SEA SSS FUL L1 (6 REACTIONS)

=> d l3 1-3

L3   ANSWER 1 OF 3 CASREACT COPYRIGHT 2007 ACS on STN

RX(6) OF 56

(step 1)
stereoisomers

16%

RX(6) OF 56

stereoisomers

REF: Carbohydrate Research, 162(2), 181-97; 1987

L3   ANSWER 2 OF 3 CASREACT COPYRIGHT 2007 ACS on STN

MeOH, SnCl2, AcCl

67%

REF: Carbohydrate Research, 25(1), 43-8; 1972
NOTE: Classification: Heterocycle formation; Ring cleavage; Hydrolysis;
      Alkoxylation; # Conditions: SnCl2 AcCl; Rf 200mn; # Comments:
      yield for alpha anomer of 5-membered ring. 14% yield for; beta
      anomer. 6% yield for alpha anomer of 6-membered ring; product.
      8% yield for beta anomer

L3   ANSWER 3 OF 3   CASREACT   COPYRIGHT 2007 ACS on STN

RX(1) OF 1

MeOH, HCl

100%

REF: Chemical Communications (London), (14), 808-9; 1968
NOTE: Classification: Alkoxylation; Acetalisation; Ring contraction; #
      Conditions: MeOH HCl 6mn 20 deg; # Comments: alpha/beta=1/1 for
      product

=> d his

     (FILE 'HOME' ENTERED AT 15:44:45 ON 12 JUN 2007)

     FILE 'CASREACT' ENTERED AT 15:44:56 ON 12 JUN 2007
L1   STRUCTURE UPLOADED
L2   0 S L1
L3   3 S L1 FULL

=>

---Logging off of STN---

=>
Executing the logoff script...

=> LOG Y

=>
Uploading C:\Program Files\Stnexp\Queries\10578800\reaction iv to v.str

chain nodes :
6   7   8   9   10 11 12 18 19 20 21 22 23 24 25 26
ring nodes :
1   2   3   4   5   13 14 15 16 17
chain bonds :
1-9 3-6 5-8 6-7 8-12 9-10 9-11 13-21 15-18 17-20 18-19 20-24 21-22 21-23 21-26 23-25
ring bonds :
1-2 1-5 2-3 3-4 4-5 13-14 13-17 14-15 15-16 16-17
exact/norm bonds :
1-2 1-5 2-3 3-4 3-6 4-5 5-8 9-11 13-14 13-17 14-15 15-16 15-18 16-17 17-20 21-23
exact bonds :
1-9 6-7 8-12 9-10 13-21 18-19 20-24 21-22 21-26 23-25

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS
 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS
 24:CLASS 25:CLASS 26:CLASS
fragments assigned product role:
containing 13
fragments assigned reactant/reagent role:
containing 1

L1   STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1   STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

```
=> s ;1
ENTER LOGIC EXPRESSION, QUERY NAME, OR (END):end
SEARCH ENDED BY USER


L2       407826 1

=> s l1
SAMPLE SEARCH INITIATED 16:48:44 FILE 'CASREACT'
SCREENING COMPLETE -    1397 REACTIONS TO VERIFY FROM      100 DOCUMENTS

100.0% DONE   1397 VERIFIED      0 HIT RXNS                 0 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED VERIFICATIONS:    25700 TO    30180
PROJECTED ANSWERS:              0 TO        0

L3            0 SEA SSS SAM L1 (     0 REACTIONS)

=> s l1 full
FULL SEARCH INITIATED 16:48:49 FILE 'CASREACT'
SCREENING COMPLETE -   32058 REACTIONS TO VERIFY FROM     1917 DOCUMENTS

100.0% DONE   32058 VERIFIED      1 HIT RXNS                 1 DOCS
SEARCH TIME: 00.00.03

L4            1 SEA SSS FUL L1 (     1 REACTIONS)

=> d l4

L4   ANSWER 1 OF 1  CASREACT  COPYRIGHT 2007 ACS on STN

RX(3) OF 24
```



```
                1. NaOH, NaBH4, Water
                2. HCl, Water
     (step 1)                              78%
REF:  PCT Int. Appl., 2005044832, 19 May 2005
CON:  STAGE(1) room temperature -> 0 deg C; <15 deg C; 30 minutes,
          cooled
      STAGE(2) pH 7



=>

---Logging off of STN---



=>
Executing the logoff script...


=> LOG Y

COST IN U.S. DOLLARS                      SINCE FILE    TOTAL
                                            ENTRY      SESSION
FULL ESTIMATED COST                        118.78      118.99

STN INTERNATIONAL LOGOFF AT 16:49:38 ON 12 JUN 2007
```

=>
Uploading C:\Program Files\Stnexp\Queries\10578800\reaction III to IV.str

chain nodes :
6   7   8   9   10   11   12   13   14   15   21   22   23   24   25   26   27
ring nodes :
1   2   3   4   5   16   17   18   19   20
chain bonds :
1-9   3-6   5-8   6-7   8-15   9-10   9-12   10-11   11-14   12-13   16-24   18-21   20-23   21-22   23-27   24-25
24-26
ring bonds :
1-2   1-5   2-3   3-4   4-5   16-17   16-20   17-18   18-19   19-20
exact/norm bonds :
1-2   1-5   2-3   3-4   3-6   4-5   5-8   9-12   10-11   16-17   16-20   17-18   18-19   18-21   19-20   20-23   24-26
exact bonds :
1-9   6-7   8-15   9-10   11-14   12-13   16-24   21-22   23-27   24-25

Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:CLASS   7:CLASS   8:CLASS   9:CLASS   10:CLASS   11:CLASS   12:CLASS
 13:CLASS   14:CLASS   15:CLASS   16:Atom   17:Atom   18:Atom   19:Atom   20:Atom   21:CLASS   22:CLASS   23:CLASS
 24:CLASS   25:CLASS   26:CLASS   27:CLASS
fragments assigned product role:
containing 16

L1   STRUCTURE UPLOADED

=> s l1
SAMPLE SEARCH INITIATED 16:45:06 FILE 'CASREACT'
SCREENING COMPLETE -   375 REACTIONS TO VERIFY FROM   18 DOCUMENTS

100.0% DONE   375 VERIFIED   0 HIT RXNS   0 DOCS
SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS: ONLINE   **COMPLETE**
                         BATCH   **COMPLETE**
PROJECTED VERIFICATIONS: 6339 TO   8661
PROJECTED ANSWERS: 0 TO   0

L2   0 SEA SSS SAM L1 (0 REACTIONS)

```
=> s l1 full
FULL SEARCH INITIATED 16:45:12 FILE 'CASREACT'
SCREENING COMPLETE -     7002 REACTIONS TO VERIFY FROM        321 DOCUMENTS

100.0% DONE     7002 VERIFIED       4 HIT RXNS                     3 DOCS
SEARCH TIME: 00.00.05

L3              3 SEA SSS FUL L1 (      4 REACTIONS)

=> d l3 1-3
```

L3   ANSWER 1 OF 3   CASREACT   COPYRIGHT 2007 ACS on STN

RX(2) OF 24

REF: PCT Int. Appl., 2005044832, 19 May 2005
CON: STAGE(1) <0 deg C; 30 minutes, <10 deg C

L3   ANSWER 2 OF 3   CASREACT   COPYRIGHT 2007 ACS on STN

RX(2) OF 15

REF: Carbohydrate Research, 181,, 125-34; 1988

L3   ANSWER 3 OF 3   CASREACT   COPYRIGHT 2007 ACS on STN

RX(2) OF 39

REF: Journal of the American Chemical Society, 107(18), 5283-5; 1985


```
=> file caplus
COST IN U.S. DOLLARS                        SINCE FILE      TOTAL
                                            ENTRY           SESSION
FULL ESTIMATED COST                         122.13          122.34

FILE 'CAPLUS' ENTERED AT 16:45:29 ON 12 JUN 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)
```

```
FILE COVERS 1907 - 12 Jun 2007  VOL 146 ISS 25
FILE LAST UPDATED: 11 Jun 2007  (20070611/ED)
```

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

```
=> s 13
L4            3 L3

=> d 14 1-3 ibib hitstr
```

L4   ANSWER 1 OF 3   CAPLUS   COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:429422   CAPLUS
DOCUMENT NUMBER: 142:463961
TITLE: Process for the preparation of 1-chloro-3,5-di-O-acyl-
                            2-deoxy-L-ribofuranoside derivatives from
                            2-deoxy-D-galactose via stereoselective chlorination
                            reaction
INVENTOR(S):   Tamerlani, Giancarlo; Bartalucci, Debora; Salsini,
                            Liana; Rapaccini, Silvia
PATENT ASSIGNEE(S):   Inalco S.p.A., Italy
SOURCE: PCT Int. Appl., 17 pp.
                            CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

```
      PATENT NO.          KIND   DATE       APPLICATION NO.       DATE
      ---------------     ----   --------   --------------------  --------
      WO 2005044832       A1     20050519   WO 2004-EP52900       20041110
          W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
              CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
              GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
              LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
              NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
              TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
          RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
              AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
              EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO,
              SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,
              NE, SN, TD, TG
      CA 2545437          A1     20050519   CA 2004-2545437       20041110
      EP 1699805          A1     20060913   EP 2004-818161        20041110
          R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
              IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS
      CN 1878782          A      20061213   CN 2004-80033026      20041110
      JP 2007510696       T      20070426   JP 2006-538856        20041110
      US 2007083041       A1     20070412   US 2006-578800        20060509
PRIORITY APPLN. INFO.:                      IT 2003-FI288     A   20031110
                                            WO 2004-EP52900   W   20041110
```
OTHER SOURCE(S):   CASREACT 142:463961; MARPAT 142:463961
REFERENCE COUNT: 1   THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS
                                  RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4   ANSWER 2 OF 3   CAPLUS   COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1989:173573   CAPLUS
DOCUMENT NUMBER: 110:173573
TITLE: Synthesis of 2-deoxy-D-arabino-(6-13C)hexose
AUTHOR(S):   Walker, Thomas E.; Ehler, Deborah S.; Unkefer,
                            Clifford J.
CORPORATE SOURCE: Los Alamos Natl. Lab., Los Alamos, NM, 87545, USA
SOURCE: Carbohydrate Research (1988), 181, 125-34
                            CODEN: CRBRAT; ISSN: 0008-6215
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S):   CASREACT 110:173573

L4   ANSWER 3 OF 3   CAPLUS   COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1985:560278   CAPLUS
DOCUMENT NUMBER: 103:160278
TITLE: Total synthesis of the cytochrome P-450 epoxygenase
                            metabolites 5(R),6(S)-, 5(S),6(R)-, and
                            14(R),15(S)-epoxyeicosatrienoic acid (EET) and
                            hydration products 5(R),6(R)- and 14(R),15(R)-
                            dihydroxyeicosatrienoic acid (DHET)
AUTHOR(S):   Moustakis, Christine A.; Viala, Jacques; Capdevila,
                            Jorge; Falck, J. R.
CORPORATE SOURCE: Health Sci. Cent., Univ. Texas, Dallas, TX, 75235, USA
SOURCE: Journal of the American Chemical Society (1985),
                            107(18), 5283-5
                            CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English

OTHER SOURCE(S):   CASREACT 103:160278

=>

---Logging off of STN---

=>
Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	4.01	126.35

STN INTERNATIONAL LOGOFF AT 16:46:12 ON 12 JUN 2007